NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

MULTIDISCIPLINARY RESEARCH GRANT

NGL 11-002-018

GEORGIA INSTITUTE OF TECHNOLOGY

FINAL REPORT

Report Prepared by

A. L. Ducoffe, Chairman

Georgia Tech Space Sciences Technology Board

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GEORGIA INSTITUTE OF TECHNOLOGY
Atlanta, Georgia 30332

Office of
The Vice President for
Academic Affairs

April 15, 1971

Dr. Francis B. Smith
Assistant Administrator for
University Affairs
National Aeronautics and Space
Administration
Washington, D. C. 20546

SUBJECT: Final Report
Multidisciplinary Research Grant NGL 11-002-018

Dear Dr. Smith:

The Georgia Institute of Technology Space Sciences and Technology Board is pleased to submit herewith thirty (30) copies of the final report for Multidisciplinary Research Grant NGL 11-002-018.

We shall be pleased to provide any additional information that you find necessary.

Sincerely yours,

Vernon Crawford

V. Crawford
Vice President for
Academic Affairs

VC/af

Enclosures

cc: Mr. H. L. Baker
Members of the Space Sciences and Technology Board

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FINAL REPORT

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

MULTIDISCIPLINARY RESEARCH GRANT NGL 11-002-018

GEORGIA INSTITUTE OF TECHNOLOGY

I. SUMMARY

The National Aeronautics and Space Administration granted the Georgia Institute of Technology $600,000 on June 15, 1964, $300,000 on June 15, 1965, $300,000 on March 15, 1966, $300,000 on March 15, 1967, and $100,000 on March 15, 1968 for the support over six years and nine months of basic scientific research entitled "Multidisciplinary Research in the Space Sciences and Technology."

The grant funds have been used to support an expansion of multidisciplinary research programs in materials and materials processing, transport phenomena, energy conversion, systems, and nuclear processes.

The grant has been administered by the Space Sciences and Technology Board established at the Georgia Institute of Technology. The Chairman of the Board is Dr. A. L. Ducoffe, Director of the School of Aerospace Engineering. The other Board members are H. F. Bauer, Engineering Mechanics; C. H. Braden, Physics; W. O. Carlson, Mechanical Engineering; J. W. Hooper, Electrical Engineering; R. H. Kasriel, Mathematics; P. Kelly, Social Sciences; H. A. McGee, Jr., Chemical Engineering; and W. M. Spicer, Director, School of Chemistry.

The last grant period runs from March 15, 1970 through March 14, 1971. The present document reports the research results obtained during the last six months of this period.

An indication of the research activity stimulated by the grant during this reporting period is the publication in recognized journals of 5 papers and the submission of 3 additional. Two papers have been read at scientific meetings. During the present grant period 1 Masters student and 12 Ph.D. students participated in the research effort.

II. RESEARCH RESULTS

1. Vibration and Stability of Distensible Fluid Lines Carrying a Pulsating Incompressible Liquid - H. F. Bauer

Objectives of Research: The feedline system of liquid propelled space vehicles exhibits a peculiar interaction with the combustion and pump dynamics and the elastic structure. The problem occurs also in pressure fed systems, where no cavitation bubbles are present in the feedline. For the speed of propagation in the liquid of $c = \infty$, i.e., incompressible liquid, as it occurs in a pressure-fed system, the propagation of viscous liquid in an elastic cylindrical pipeline has been investigated.

Description of the Work Performed: The pulsating flow of an incompressible, viscous liquid in an elastic pipeline of circular cross section has been investigated for small displacements and velocities. The linearized basic equations are (because of symmetry) given by:

The equation of continuity:

$$\frac{\partial u}{\partial r} + \frac{u}{r} + \frac{\partial w}{\partial z} = 0 \tag{1}$$

The Navier-Stokes equations for incompressible flow:

$$\frac{\partial u}{\partial t} = + \nu\left[\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} - \frac{u}{r^2} + \frac{\partial^2 u}{\partial z^2}\right] \tag{2}$$

$$\frac{\partial w}{\partial t} = - \frac{1}{\rho}\frac{\partial p}{\partial z} + \nu\left[\frac{\partial^2 w}{\partial r^2} + \frac{1}{r}\frac{\partial w}{\partial r} + \frac{\partial^2 w}{\partial z^2}\right] \tag{3}$$

The behavior of the elastic cylindrical pipeline of infinite length is described by Donnell's shell equations:

$$\frac{\bar{\nu}}{a}\frac{\partial \bar{w}}{\partial z} + \frac{\bar{u}}{a^2} + \frac{h^2}{12}\frac{\partial^4 \bar{u}}{\partial z^4} + \frac{(1-\bar{\nu}^2)}{E}\bar{\rho}\frac{\partial^2 \bar{u}}{\partial t^2} = \frac{(1-\bar{\nu}^2)}{E\bar{h}}\left\{p\Big|_{r=a} - 2\mu\frac{\partial u}{\partial r}\Big|_{r=a}\right\} \tag{4}$$

$$\frac{\partial^2 \bar{w}}{\partial z^2} + \frac{\bar{\nu}}{a}\frac{\partial \bar{u}}{\partial z} - \frac{(1-\bar{\nu}^2)}{E}\rho\frac{\partial^2 \bar{w}}{\partial t^2} = \frac{(1-\bar{\nu}^2)}{E\bar{h}}\mu\left[\frac{\partial u}{\partial z} + \frac{\partial w}{\partial r}\right]_{r=a} \tag{5}$$

The equations of motion of the liquid and elastic pipeline are coupled through the conditions

$$u = \frac{\partial \bar{u}}{\partial t} \quad \text{and} \quad w = \frac{\partial \bar{w}}{\partial t} \quad \text{at the wall } r=a. \tag{6}$$

Representing the pressure and velocities as

$$p = \frac{P_o}{2} z + \mathrm{Re}\left[\sum_{n=1}^{\infty} \left\{ P^*_{1n} \, e^{i\omega \, n(t-z/c_n)} + P_{2n} \, e^{i\omega \, n(t+z/c_n)} \right\} \right] \qquad (7)$$

with

$$P^*_{1n} = P_{1n} - i\bar{P}_{1n}$$

$$P^*_{2n} = P_{2n} - i\bar{P}_{2n}$$

where ω is the circular frequency and c_n is the speed of propagation, yields with:

$$u = \mathrm{Re}\left[\sum_{n=1}^{\infty} \left\{ U^*_{1n}(r) \, e^{i\omega \, n(t-z/c_n)} + U^*_{2n}(r) \, e^{i\omega \, n(t+z/c_n)} \right\} \right] \qquad (8)$$

and

$$w = \frac{W_o}{2} + \mathrm{Re}\left[\sum_{n=1}^{\infty} \left\{ W^*_{1n}(r) \, e^{i\omega \, n(t-z/c_n)} + W^*_{2n}(r) \, e^{i\omega \, n(t+z/c_n)} \right\} \right] \qquad (9)$$

the equations:

$$W_o'' + \frac{1}{r} W_o' = \frac{P_o}{\mu} \qquad (10)$$

and

$$U^{*\prime}_{\lambda n} + \frac{1}{r} U^{*}_{\lambda n} = \pm \frac{2n\omega W^{*}_{\lambda n}}{c_n} \tag{11}$$

$$U^{*\prime\prime}_{\lambda n} + \frac{1}{r} U^{*\prime}_{\lambda n} + \left(k_n^2 - \frac{1}{r^2}\right) U^{*}_{\lambda n} = 0 \tag{12}$$

$$W^{*\prime\prime}_{\lambda n} + \frac{1}{r} W^{*\prime}_{\lambda n} + k_n^2 W^{*}_{n\lambda} = \mp \frac{in\omega}{\mu c_n} P^{*}_{\lambda n} \tag{13}$$

where $k_n^2 = \frac{i^3\omega n}{\nu} - \frac{\omega^2 n^2}{c_n^2}$ and the upper sign belongs to $\lambda=1$, while the lower sign belongs to $\lambda=2$, the reflected waves. They are satisfied for $\omega^2 n^2 \ll c_n^2$ by

$$W_o(r) = \frac{P_o a^2}{4\mu}\left(1 - \frac{r^2}{a^2}\right) \qquad \text{(Poiseuille Flow)} \tag{14}$$

and

$$W^{*}_{\lambda n}(r) = A_{\lambda n} J_o(k_n r) \mp \frac{i\omega n}{\mu c_n k_n^2} P^{*}_{\lambda n} \tag{15}$$

$$U^{*}_{\lambda n}(r) = \frac{i\omega n}{c_n k_n} A_{\lambda n} J_1(k_n r) + \frac{\omega^2 n^2 r}{2\mu c_n^2 k_n^2} P^{*}_{\lambda n} \tag{16}$$

where $A_{\lambda n}$ are unknown integration constants. The elastic wall equations are with

$$\bar{u} = \frac{\bar{u}_o}{2} + \mathrm{Re}\left[\sum_{n=1}^{\infty} \left\{ \bar{U}^*_{1n} \, e^{i\omega \, n(t-z/c_n)} + \bar{U}^*_{2n} \, e^{i\omega \, n(t+z_o/c_n)} \right\} \right] \tag{17}$$

$$\bar{w} = \mathrm{Re}\left[\sum_{n=1}^{\infty} \left\{ \bar{W}^*_{1n} \, e^{i\omega \, n(t-z/c_n)} + \bar{W}^*_{2n} \, e^{i\omega \, n(t+z_o/c_n)} \right\} \right] \tag{18}$$

given by:

$$\left(\bar{U}_o = \frac{(1-\bar{\nu}^2) a^2}{E\bar{h}} \, P_o \right).$$

$$\bar{U}^*_{\lambda n} \left[\frac{1}{a^2} - \frac{(1-\bar{\nu}^2)}{E} \rho \omega^2 n^2 \right] - \frac{\nu i \omega n}{a c_n} \bar{W}^*_{\lambda n} = \frac{(1-\bar{\nu}^2)}{E\bar{h}} \left[P^*_{n\lambda} - 2\mu \left\{ \frac{i\omega n A_{\lambda n}}{c_n} J_1'(k_n a) + \frac{\omega^2 n^2 P^*_{\lambda n}}{2\mu c_n^2 k_n^2} \right\} \right] \tag{19}$$

and

$$- \frac{i\omega n\bar{\nu}}{ac_n} \bar{U}^*_{\lambda n} + \bar{W}^*_{\lambda n}\left[\frac{(1-\bar{\nu}^2)\rho\omega^2}{E} - \frac{\omega^2 n^2}{c_n^2}\right] = \frac{(1-\nu^2)}{E\bar{h}} \mu\Big[i\omega n \left\{\frac{i\omega n A_{\lambda n}}{c_n k_n} J_1(k_n a)\right. \quad (20)$$

$$\left. + \frac{\omega^2 n^2 a^2 P^*_{\lambda n}}{2\mu c_n^2 k_n^2}\right\} + A_{\lambda n} k_n J_o'(k_n a)\Big]$$

With the boundary conditions (6) one obtains two additional equations

$$\frac{in\omega}{c_n k_n} J_1(k_n a) + \frac{\omega^2 n^2 a P^*_{\lambda n}}{2\mu c_n^2 k_n^2} = i\omega n \bar{U}^*_{\lambda n} \quad (21)$$

$$aJ_o(k_n a) - \frac{i\omega n P^*_{\lambda n}}{\mu c_n k_n^2} = i\omega n \bar{W}^*_{\lambda n} \quad (22)$$

Together with equations (19) and (20) these represent four equations for the determination of the unknowns. The speed of propagation c_n is obtained by setting the determinant equal to zero. From the above equations (19) through (22) the ratios $A_{\lambda n}/P^*_{\lambda n}$, $\bar{U}^*_{\lambda n}/P^*_{\lambda n}$ and $\bar{W}^*_{\lambda n}/P^*_{\lambda n}$ may be obtained, and are given as functions of the system parameters. Introducing these into the equations (7), (8), (9), (17) and (18) yields the results of the behavior of such a pulsating system, superimposed upon a uniform flow (14).

Results: The mathematical solution has been found for an arbitrarily pulsating flow superimposed upon a uniform flow. The speed

of propagation c_n is obtained by setting the coefficient determinant obtained from equations (19) through (22) equal to zero. With this the ratios $A_{\lambda n}/P^*_{\lambda n}$, $\bar{U}^*_{\lambda n}/P^*_{\lambda n}$ and $\bar{W}^*_{\lambda n}/P^*_{\lambda n}$ are obtained from these equations. The values $A_{\lambda n}$, $\bar{U}^*_{\lambda n}$ and $\bar{W}^*_{\lambda n}$ are therefore known for a given pressure.

Publication: "On the Shape of a Rotating Fluid System Consisting of a Gas Bubble Enclosed in a Liquid Globe," Zeitschrift fur Angewandte Mathematik und Physik. (Accepted for Publication)

Graduate Student: Ph.D. Candidate.

2. A Study of Helicopter Blade Slap Noise - R. B. Gray

Research Performed and Results Obtained: The interaction under certain flight conditions of a helicopter blade with the vortex field shed from preceeding blades produces a loud repetitive noise. Other studies have shown that a realistic mathematical model of the vortex structure is required for analysis of the noise generating mechanism. Such a model is not presently available. The objective of this grant is to explore several methods of measuring the flow field associated with vortex systems.

Thus far, a hot-wire anemometer has been used to study the flow field of vortex rings generated in air. By suitable orientation of the single wire, magnitudes of the total velocity and the axial velocity have been obtained across the vortex at a station 0.3 meters from the vortex generator exit. During this reporting period, a hot-film vector anemometer has been acquired which is capable of measuring the three velocity components simultaneously. The output of this vector

anemometer will be fed into a small digital computer for data reduction. The computer program has been written and checked out. The electronic interface including the analog to digital converters have also been designed, assembled, and checked out. It is conservatively estimated that the system is capable of a velocity vector sampling rate greater than ten thousand per second. This will be used for further study of the vortex ring.

The helicopter model rotor test facility is in the detail design stage. Construction is expected to begin in the near future.

A proposal has been written and submitted to NASA Langley to study vortex shedding from helicopter blades.

Graduate Student: M.S. Student.

3. Energy Conversion in Reactive Collisions - T. Moran

Research Performed and Results Obtained: As part of the program in High Energy Chemistry we have pursued the experimental and theoretical aspects of our investigations into the fundamental basis of energy conversion in reactive and non-reactive bimolecular collisions. Ion-molecule reactions have been examined in a significantly improved high resolution beam apparatus. Reactant ion beams are supplied by a small Nier type mass spectrometer. The ion beams from this spectrometer are focused into a 127° electrostatic energy selector which was fabricated from fine wire mesh grids of a design similar to those used in electron scattering experiments. The mass and energy selected ion beam is then focused into the collision chamber where reactions take place. Neutral

target molecules enter the collision region through a multichannel, fused capillary array which provides high target atom concentrations in a small, well defined region with a primarily monodirectional velocity distribution. This neutral beam, which intersects the ion beam in a perpendicular direction, is fed directly into a 3000-l/sec. diffusion pump. Ionic scattering products are measured in the out of plane dimension with a detection system consisting of another 127° sector, a Paul-Steinwedel mass filter and a channel electron multiplier. Channeltron signal pulses are amplified, shaped and then counted. The entire apparatus is mounted on an optical bench inside a 32 in. diameter stainless steel high vacuum chamber.

In ion-neutral molecule scattering processes, the kinetic energy of elastically scattered ions can be calculated from the expression

$$E_e = \frac{M^2 E_o}{(m+M)^2}\left[(2\cos^2\theta - 1) + \left(\frac{m}{M}\right)^2 \pm \frac{2m}{M}\cos\theta\left(1-\frac{M^2}{m^2}\sin^2\theta\right)^{1/2}\right]$$

where θ is the laboratory scattering angle, E_o is the energy of the incident ion of mass M and m is the mass of the target atom. For inelastically scattered ions a similar relation holds

$$E_i = \frac{M^2}{(M+m)^2}E_o\left[(2\cos^2\theta - 1) + \frac{m^2}{M^2}\left(1-\frac{\Delta E}{E_s}\right) \pm \frac{2m}{M}\left(1-\frac{\Delta E}{E_s}\right)^{1/2}\cos\theta\left(1-\frac{M^2\sin^2\theta}{m^2\left(1-\frac{\Delta E}{E_s}\right)}\right)^{1/2}\right]$$

where ΔE is the spectroscopic energy loss and E_e is equal to $mE_o/(m+M)$. The kinetic energy distribution of the primary ion beam approximates 0.04 eV FWHM which is sufficiently narrow to allow separation of the elastic and inelastic components of the scattered beam. A convenient measure of inelasticity, or degree of energy conversion, is given by E_e-E_i which can be computed knowing the energy of the incident ion, masses of reactants, the scattering angle θ and ΔE computed from spectroscopic constants using the relation

$$\Delta E = hc\omega_e(\nu'-\nu) - hc\omega_2 X_e\left[(\nu'+1/2)^2-(\nu+1/2)^2\right]+(h^2/8\pi^2 I)\left[J'(J'+1)-J(J+1)\right]$$

where primed numbers refer to the final quantum states. The inelastic energy loss spectra for a typical interaction of the type

$$CO^+X^2\sum(\nu,J) + Ar \rightarrow CO^+X^2\sum(\nu',J') + Ar$$

show that the majority of inelastically scattered product ions are forward scattered with positions approximating those from the computed values of E_e-E_i. Experimental points at large angles give evidence of rather sharp peaks due to inelastic collisions corresponding to vibrational excitations but at smaller angles there is significant broadening of these peaks and at nominal 0° LAB angle a maximum appears in the scattered intensity below the $\nu=0\rightarrow1$ threshold. Although a small amount of inelastic peak broadening is expected from the finite velocity width of the incident ion beam and small out of plane velocity components of

the target atoms; the experimental width of the inelastic peaks is larger than expected for pure vibrational transitions and gives indications of simultaneous vibrational and rotational excitations. As the reactant ion kinetic energy is lowered to 3 eV LAB energy, transitions with smaller energy losses become relatively more important and correspond to pure rotational excitations with changes in rotational quantum number, $\Delta J \approx 20$ for these large impact parameter collisions.

The relative differential cross sections measured for the vibrational excitations compare favorably with those predicted from a forced harmonic oscillator model with time dependent wavefunctions to evaluate transition probabilities. This model correctly predicts the relative $\nu = 0 \rightarrow n$ vibrational cross sections at given values of LAB scattering angles and the angular variation of these cross sections once the interaction potential has been determined.

The energy conversion processes involving chemically reactive species have been examined and it is found that a statistical model adequately describes total cross sections for various reaction channels as a function of incident ion translational energy. The cross sections for chemical rearrangement reactions of low energy C^+ ions with N_2 and O_2 leading to CN^+ and CO^+ respectively, are in reasonable agreement with the predictions of the statistical phase space model as regards translational energy dependences. However quantitative comparison between the results using this model and experimental data indicate that product states do not necessarily mix statistically and spin and symmetry requirements play a role in determining the product states. Translational energy dependences of dissociative reactions as determined from the

statistical model appear to be correct, but the statistical treatment overestimates the magnitude of this channel. Competing charge transfer processes with close energy balance between initial and final states, are better described by the nearest resonance model with the statistical approach limited to close coupled collisions where the electron transfer reactions have significant energy defects.

Publications: "Pure Rotational Excitation in CO^+ - Ar Interactions by Ion Beam Collision Spectroscopy," T. F. Moran, Frederick Petty and George S. Turner, Submitted to Chemical Physics Letters.

"Calculated Ion-Molecule Reactions of C^+ with O_2 and N_2," D. C. Fullerton and T. F. Moran, Submitted to International Journal of Mass Spectrometry and Ion Physics.

"Vibrationally Inelastic, Low Energy CO^+ - Ar Collisions," F. C. Petty and T. F. Moran, Submitted to Physical Review.

Papers Presented to Scientific Meetings: An invited paper "Vibrational Excitation in the Collisions of Atomic Ions with Neutral Molecules" will be presented in July at the Cambridge Conference on Molecular Energy Transfer, which is jointly sponsored by Cambridge University, England, and the U. S. National Academy of Sciences.

Graduate Students: Two Ph.D. Students.

4. Atomic and Magnetic Ordering in Transition Metal Alloys - S. S. Spooner

Summary of Progress: The electronic structure of the magnetic moments in the equiatomic alloys has been under investigation by polarized

neutron diffraction as a function of order and the metallurgical aspects of vanadium alloys additions have been under metallographic study in an attempt to understand the commercial practice of alloying the equiatomic alloys with 2% V. Recent band calculations for pure iron (Duff and Das, Phys. Rev. 3, 192 (1971)) provide important insights into the electronic structure which allow us to conclude that our results from Mossbauer spectroscopy and neutron diffraction experiments are consistent. The metallurgical question is far from being completely understood, but it can be suggested that interstitial impurity control and grain refinement effects due to vanadium may serve as an important additional factor in inhibiting brittle fracture tendency in the commercial FeCo alloy.

The polarized neutron diffraction experiments on polycrystalline alloys in the ordered and disordered condition give an indication of the changes in electron structure as a function of order. The magnetic electron form factors which are experimentally measured are related to the Fourier transform of the magnetic electron density and in other experiments on metals have been analyzed in terms of calculated form factors derived from free atom calculations by Watson and Freeman. In consideration of the fact that we are in fact dealing with atoms in the metallic state, it is very fortunate that the free atom calculations are found to be so useful. Our most recent efforts in data analysis show that the cobalt magnetic moment undergoes an apparent change in spacial distribution which is indicated by the fact that use of the Co^{+3} form factor in the ordered state and Co^{+1} form factor in the disordered state lead to the best data fit. The Fe^{+2} form factor appears

to apply in both ordered and disordered states. Using this kind of form factor analysis, it is found that the localized magnetic moments on iron or on cobalt do not change as drastically as we first thought. However, the unlocalized magnetization is negatively polarized and decreases in magnitude upon ordering. (This determination is based on demanding a consistency between bulk magnetization and localized magnetization determined in the neutron scattering experiments.)

In addition to assessing the magnitude of moments, we obtained a measure of the non-spherical distribution of the local moment electrons which is due to the cubic crystalline field. The degree of asphericity observed in the magnetic electron form factors was comparable to the asphericity observed in pure iron and was not a function of order in the alloy.

The changes in the magnetic electron structure are indicated in Mossbauer spectroscopy through changes in hyperfine field and changes in polarized electron density at the iron nucleus giving an isomer shift. The decrease in the negative magnitude of the hyperfine field upon ordering is consistent with our neutron observations of the moment changes using the view that the dipolar effects of the cobalt moment at the iron nucleus play the prominant role. However, the negatively polarized non-localized moment was found to decrease in magnitude upon ordering, making it difficult to explain the change of isomer shift with ordering which would call for an increase in negatively polarized electron density at the nucleus. It has been suggested by many that the non-localized electrons were s-like in character. However, the calculations for pure iron by Duff and Das appear to offer a means for rationalizing

our observations. They show that the negative magnetization density associated with non-local electrons is found in outlying regions of the atomic cell and is due to spin dependence of the radial part of the d-electron wave functions. Furthermore, there appears to be no mechanism for negative polarization of the 4-s electron wave function in iron. Thus, no direct connection between non-localized moment and 4-s electron wave functions is required by their model of electron behavior for iron.

The further analysis of the ordering changes upon the electronic structure through magnetic electron behavior appears to be a promising approach.

The metallurgical aspects of alloying additions to iron-cobalt in order to control brittleness have been controversial for some time. On one hand, it has been advocated that control of ordering by alloying additions was principally responsible for mechanical property improvement. On the other hand, interstitial impurity effects on embrittlement are thought to be controlled by vanadium as a gettering agent. It would be surprising if both views were not correct in some degree.

The effect of carbon in the iron-cobalt system was put under study since carbides can play an important role in brittle fracture. A pure iron, an iron-cobalt, and a commercial Fe-Co-2%V alloy were carburized at 950°C and then rapidly cooled and metallographically polished to reveal carbide structure. While the treatment was in no way representative of industrial practice to our knowledge, it afforded a convenient means for examining carbide behavior in iron-cobalt and iron-cobalt alloys. Two features in this study were revealed metallographically:

1) carbide formation morphology differences, and

2) vanadium carbide inhibition of grain growth and cementite growth.

The vanadium carbide precipitation at austenite grain boundaries as well as within grains appeared to confine carbide formation to a continuous mode of precipitation (as distinguished from a discontinuous-cellular mode). Small austenite grain size was preserved in the vanadium containing alloy while a larger grain size in both iron and iron-cobalt developed in the early stages of carburization treatment. The mode of carbide precipitation in Fe-Co was distinctly different from the well known pearlite formation, but macroscopically resembled a plate-like growth with irregular though nearly parallel boundaries between the body-center cubic ferrite and carbide cementite.

It is known that cobalt carbide is highly unstable and that graphite precipitation is favored in cobalt containing alloys. With this in mind we were interested in learning whether cobalt was equally partitioned between the ferrite and carbide. Our microprobe studies are not complete although it can be anticipated that in the first of our experiments with rapid formation of carbide, substitutional diffusion would not allow much adjustment of cobalt content in the carbide. Nevertheless, it is interesting to note that the mode of carbide formation is distinctly different between the iron and the iron-cobalt case. Whether this is due to an increase in the eutectoid temperature with cobalt additions (carbide precipitation starting temperature) or due to cobalt partitioning effects or due to changes in bulk and surface thermodynamic properties of the carbide is not certain.

In retrospect, our investigations have pointed out that carbide formation with vanadium will tie up carbon in a form that will prevent graphite flake formation, reduce interstitial embrittlement and inhibit grain growth. All these factors militate against brittleness and brittle fracture tendency.

Publication: "Magnetic Scattering of Neutrons by Equiatomic FeCo in the Ordered and Disordered State," by J. W. Lynn, S. Spooner and J. W. Cable, to appear in Solid State Division Report of the Oak Ridge National Laboratory (1971).

Graduate Students: Two Ph.D. Candidates.

5. The Physical and Functional Aspects of Integrated-Circuit Technology - K. L. Su and D. C. Ray

Research Performed: In the circuit phase, further work has been done in the synthesis of active networks using the positive impedance converter (PIC), resistors, and capacitors. The results of the investigation of RC-PIC synthesis can be summarized in the following theorems:

Theorem 1

For the realization of an arbitrary N x N matrix of real rational functions in the complex frequency variable as a short-circuit admittance matrix of a transformerless active RC N-port network, (a) it is, in general, necessary that the network contains N PIC's; and (b) it is sufficient that the network contains N PIC's embedded in a 3N-port RC network.

Theorem 2

For the realization of an arbitrary N x N matrix of real rational functions in the complex frequency variable as a short-circuit admittance matrix of a transformerless grounded active N-port RC network, it is sufficient that the network contains 2N PIC's embedded in a (4N+1)-terminal RC network.

Theorem 3

An N x N matrix of real rational functions in the complex frequency variable having L simple poles on the negative real axis in the complex frequency plane and no more than L+1 zeros can be realized as a short-circuit admittance matrix of a transformerless active network having no more than N PIC's embedded in a 2N-port RC network.

Theorem 4

An N x N matrix of real rational functions in the complex frequency variable having L simple poles on the negative real axis in the complex frequency plane and no more than L+1 zeros can be realized as a short-circuit admittance matrix of a transformerless grounded active network having no more than 2N PIC's embedded in a (3N+1)-terminal RC network.

Theorem 5

For the realization of an arbitrary N x N matrix of real rational functions in the complex frequency variable as a voltage transfer matrix of a transformerless active RC 2N-port network, (a) it is, in general, necessary that the network contains N PIC's; and (b) it is sufficient that the network contains N PIC's embedded in a 3N-port RC network.

Theorem 6

For the realization of an arbitrary N x N matrix of real rational functions in the complex frequency variable as a voltage transfer matrix of a transformerless grounded active RC 2N-port network, it is sufficient that the network contains 2N PIC's embedded in a (4N+1)-terminal RC network.

The results of the investigation on stability criteria reveals that if one port of a terminated PIC is open-circuit stable (OCS) and short-circuit stable (SCS), the other port must also be OCS and SCS. The conditions for the terminated PIC to be OCS and SCS are imposed on the dynamic gains of controlled sources in the PIC, which can easily be satisfied from practical points of view.

The study of the sensitivity in the RC-PIC networks with respect to the current-conversion-gain change in the PIC can be reduced drastically as compared to those in RC networks with the negative impedance converters, while sensitivities with respect to the voltage-conversion-gain change in the PIC increase slightly.

In the device phase, work has been centered on the assembly of an rf sputtering station utilizing an NRC oil diffusion pump (NHS4) fitted with a liquid nitrogen cryobaffle. Several difficulties were resolved in developing an operational system capable of sputtering semiconductor films at argon pressures of two microns.

A series of Ge films were sputtered using freshly cleaved CaF_2 as the substrate material. Electron diffraction studies indicated that good single crystal films had been obtained at substrate temperatures of 400°C. This suggests that the surface and its preparation

rather than the gross deposition parameters of the rf sputtering process itself are the major obstacles to obtaining epitaxy on sapphire.

This line of reasoning led to the design and construction of a novel substrate platform for sputter cleaning either conducting or insulating substrates. The required negative bias of a few hundred volts was developed by separate excitation at 7 MHz in order that cleaning might take place at any stage of the primary target sputtering process. The platform also incorporated a graphite cloth radiant heater and a radiantly heated thermocouple for measuring substrate temperature. A tuning network was constructed to match the glow discharge impedance of the platform to the rf exciter output impedance.

The analysis of the eddy current method of measuring film conductivity at microwave frequencies was extended to include the effects of the substrate. An Algol program was written and computations were made for germanium films on calcium fluoride and sapphire substrates. The surprising dependence of the film dissipated power upon the substrate thickness appeared to be substantiated by data from earlier experimental measurements. However further analytical and experimental investigations are required to exploit the significance of these results.

Publication: N. W. Cox, Jr., K. L. Su, and R. P. Woodward, "Operational-Amplifier Realization of the Nullor and the Universal Impedance Converter," to appear in IEEE Transactions on Circuit Theory, May 1971.

Graduate Students: Three Ph.D. Candidates.

6. Collisional De-excitation of Atomic Particles - E. W. Thomas

Research Performed in the Current Period: Work has been concentrated on the study of the cross section differential in angle for the charge transfer process. Work is principally directed at targets of helium where a theoretical understanding should be tractable; however, empirical data has also been obtained for more complex targets of practical interest.

It appears that the proportion of the neutrals formed in the 2s state is a very sensitive function of scattering angle; excited state fractions of 10% have been recorded at large angles. The proportion of metastable neutrals rises from about 1% at zero scattering angle to 10% at one degree of arc or greater angles; the rise is very rapid and occurs at approximately the same impact parameter for all impact energies. Some qualitative understanding of this phenomenon in the case of H^+ impact on He may be achieved by inspection of the potential energy curves of the $(H\ He)^+$ molecule. At the internuclear separation where the rise in probability of metastable formation occurs, one finds a fairly rapid change in the relative separation of certain important potential energy curves. At greater separations the curve for H(2s) lies much higher in energy than H(1s), implying that H(1s) formation is the most likely neutral atom formation mechanism; thus small angle scattering which must involve large internuclear separation gives rise to small probabilities of metastable formation. In contrast, at small internuclear separations the curves for H(1s) and H(2s) are very close together and one expects only small differences in cross sections for the formation of these levels; this again is consistent with the

observation that large angle scattering, which inevitably involves small internuclear separations, gives rise to a population of the metastable state that is of the same order as ground state population. While the considerations give qualitative explanations of the observed behavior, a quantitative understanding has not yet been properly developed.

The phenomena described for charge transfer in helium are repeated in the same general manner when considering heavier, more complex gas targets. In these cases, however, a detailed understanding is more difficult due to the non-availability of accurate potential curves.

The experiments have also yielded general information on scattering cross sections that may be correlated with a Rutherford type theoretical formulation and utilized to derive an effective potential for the interaction of the colliding atoms. Use of screened Coulomb potentials provides a rather good prediction of the cross section for the scattering of all particles into some definite angle.

A detailed study has also been made of processes whereby H_2^+ is dissociated and H(2s) formed. In this case one has three or more particles participating in the collision; the description of potential energy must be detailed in terms of a family of surfaces. The dissociation problem is rather complex. Here again it is observed that a small proportion of metastable neutrals is produced in small angle scattering and a large proportion at large angles. The detailed angular distribution can in part be predicted in terms of the potential energy liberated in the frame of reference of the dissociating molecule.

The work on this project will continue with particular emphasis on the study of complex target systems (O_2, N_2 and possibly O) and further studies also made on the processes whereby H(2s) is collisionally destroyed.

Publications: "Formation of Metastable Hydrogen Atoms by Charge Transfer," by R. L. Fitzwilson and E. W. Thomas will be published in the "Physical Review" (April 1971).

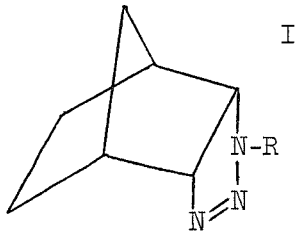
"Differential Cross Sections for the Formation of Metastable Hydrogen by Charge Transfer," by E. W. Thomas and R. L. Fitzwilson has been published in the "Bulletin of the American Physical Society" (Volume 15, page 1504, 1971).

Paper Presented to Scientific Meetings: A paper entitled "Differential Cross Sections for the Formation of Metastable Hydrogen by Charge Transfer" was presented at the "Annual Meeting of the Division of Electron and Atomic Physics of the American Physical Society" in Seattle (November 1970).

Graduate Students: Two Ph.D. Candidates.

7. Studies in Nitrene Chemistry - L. H. Zalkow and C. L. Liotta

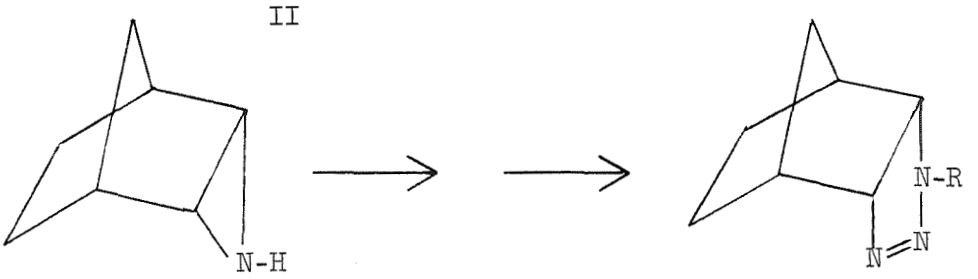
Introduction: The goal of this problem is to prepare an endo-triazoline of the bicyclo [2,2,1] System as shown.



I

In the past there have been several attempts to prepare this type of compound. To date there has been reported only one success in which phenyl azide was added to norbornene[1]. The endo adduct was prepared in low yield and was isolated via fractional crystallization from the exo isomer. A better method has yet to be reported.

Our approach to this problem is to first prepare the unsubstituted endo-aziridine II in good yield and then convert this to the desired triazoline.



There have been many attempts to add electrophilic reagents (INCO, IN_3, etc.) to norbornene in hopes to incorporate a nitrogen containing functional group endo. These have not worked at all.

There seems to be several alternatives to the above procedures. First is incorporation of the nitrogen function in the molecule at the start. Secondly, to block the exo- attack of certain reagents by placing a hindering group on the C_7 carbon syn to the double bond in norbornene. Thirdly, a sequence of reactions to convert some nitrogen function on the norbornane skeleton to an endo nitrogen functional group.

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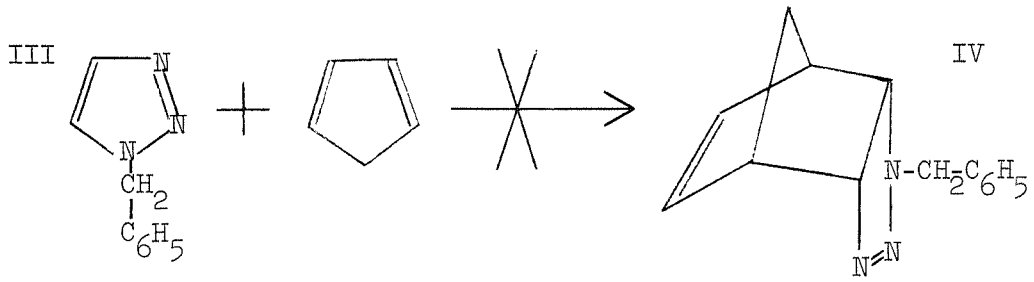
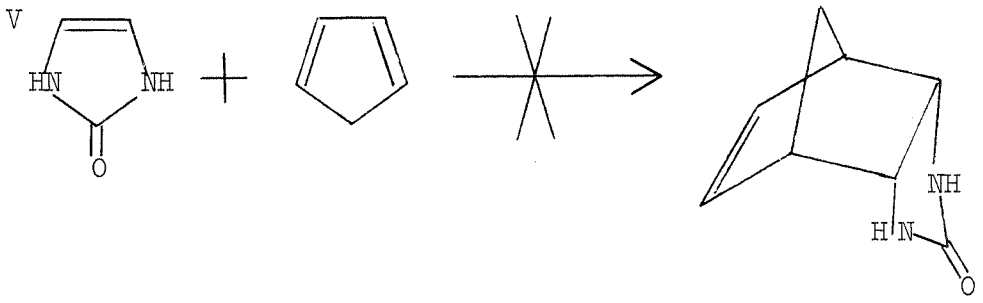
[1] S. McLean & D. M. Findlay, Tet. Letters, #27, 2219 (1969).

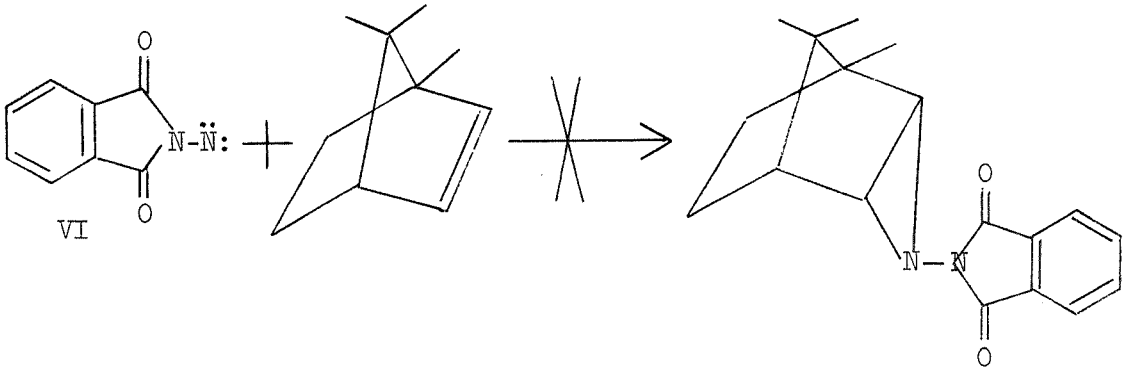
Experiments: The triazole III was prepared and attempts were made to react this with cyclopentadiene in hopes that the endo triazoline IV would form. The triazole failed to react.



The imidazolone V was prepared and attempts were made to react this with cyclopentadiene. The starting imidazolone was recovered unchanged.

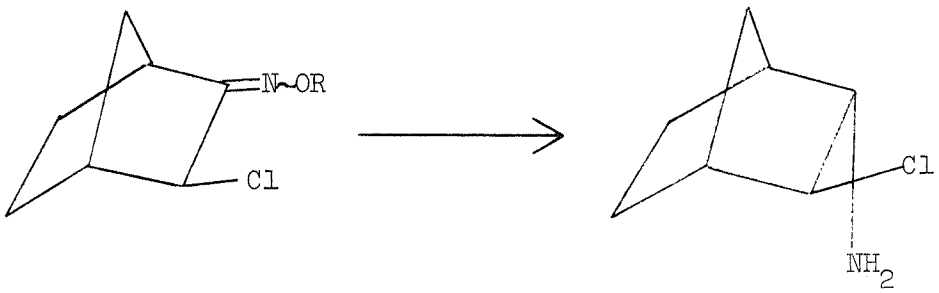


In still another attempt the nitrene VI formed from treatment of N-amino phthalimide with lead tetraacetate was added to bornylene.



There was no adduct formed.

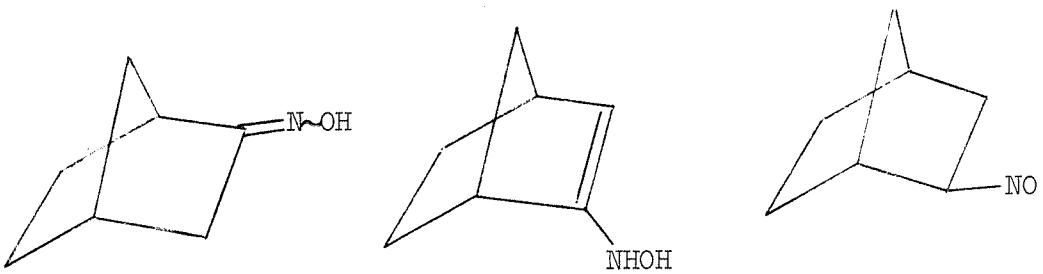
At present the best approach which is being developed in the preparation of the chlorooxime VIIa and subsequent reduction to the amino compound VIII.



VII
a,R = H
b,R = Ac

VIII

The reaction of VIIIb with $NaBH_4$ in methanol gives the dehalogenated and reduced products IX and X or XI.



IX X XI

Catalytic reduction with Rh on carbon is presently being pursued. Although no products have been identified, the resulting products seem to have been dehalogenated.

Graduate Students: Two Ph.D. Candidates.

III. CONCLUSIONS

The NASA Multidisciplinary Grant NGL 11-002-018 continued to stimulate research on the campus and its effectiveness is demonstrated by the number of publications (5), submissions (3) and presentations (2) during the six month period, September 15, 1970 to March 14, 1971.

Through the grant graduate students are engaged in quality research activities and students in the following categories received financial support from the grant: M.S. - 1 and Ph.D. - 12.